Phase Diagram and Visibility of Optically Trapped Bosons

- Optically Trapped Atoms and Boson Hubbard Model
- Matter Wave Interference Experiment
- Equilibrium Phase Diagram: Uniform System
- Equilibrium Phase Diagram: Confined System
- Visibility
- “Pause” in Evolution with $U$
- Conclusions
Collaborators

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Optical lattice in a trap

The lattice sites are the nodes of the standing wave.
Lattice spacing \( a = \lambda / 2 \)
The model

The Hamiltonian for bosonic atoms in external trap:

\[ H = \int d^3x \, \psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_0(x) + V_T(x) \right) \psi(x) \]

\[ + \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int d^3x \, \psi^\dagger(x) \psi^\dagger(x) \psi(x) \psi(x) \]

\[ \psi(x) : \text{boson field operator, } V_T(x) : \text{confining potential} \]

\[ a_s : \text{scattering length } V_0(x) : \text{optical lattice potential} \]

Simplest case:

\[ V_0(x) = \sum_{j=1}^{d} V_{j0} \sin^2(kx_j) \]

\[ k = \frac{2\pi}{\lambda} \]

\[ a = \frac{\lambda}{2} \]
The bosonic Hubbard model

Well described by the tight-binding bosonic Hubbard model,\(^1\)

\[
H = -J \sum_{\langle i,j \rangle} (b^\dagger_i b_j + b^\dagger_j b_i) + \sum_i V_T(x_i) \hat{n}_i + U \sum_i \hat{n}_i (\hat{n}_i - 1)
\]

where

\[
[b_i, b_j^\dagger] = \delta_{ij}, \quad \hat{n}_i = b_i^\dagger b_i
\]

Model parameters can be tuned.
A great deal is known about this model without trap including its phase diagram

Absorption images (in 3D) of multiple matter wave interference patterns. (a) $U = 0E_r$, (b) $U = 3E_r$, (c) $U = 7E_r$, (d) $U = 10E_r$, (e) $U = 13E_r$, (f) $U = 14E_r$, (g) $U = 16E_r$, (h) $U = 20E_r$ ($E_r = \frac{\hbar^2 k^2}{2m}$)

The claim: Quantum phase transition SF $\rightarrow$ Mott Insulator for $U \approx 12E_r$

Several recent experiments produced MI on 1D optical lattices in traps

Review 1D uniform ($V_T(x) = 0$) model
One dimensional uniform Hubbard model in the ground state$^2$

\[ H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i n_i \]

No hopping limit: $J/U = 0$

\[ H = U \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i \]

Ground state is obtained by minimizing the energy,

\[ \epsilon(n) = U n(n - 1) - \mu n \]

where $n \geq 0$ is the occupation of the site. For

\[ 2(n - 1) < \frac{\mu}{U} < 2n \]

The energy is minimized by having $n$ bosons on each site.

$\mu$ can be changed in this interval and $n$ does not change:

Excitation energy gap, incompressible Mott Insulator.

Perturbation shows that this Mott Insulator extends into the finite $J/U$ region.

World-Line Quantum Monte Carlo Simulations

Inverse Temperature discretized: \( \beta = L\Delta \tau \)

\[
Z = \text{Tr} e^{-\beta H} = \text{Tr} [e^{-\Delta \tau H}]^L
\]

Checkerboard Decomposition:
Divide Hamiltonian into two mutually commuting pieces

\[
H_a = -J \sum_{i \text{ odd}} (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + U/2 \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu/2 \sum_i \hat{n}_i
\]

\[
H_b = -J \sum_{i \text{ even}} (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + U/2 \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu/2 \sum_i \hat{n}_i
\]

Insert complete sets of occupation number states

\[
Z = \sum_{n_l} \langle n_0 | e^{-\Delta \tau H_a} | n_1 \rangle \langle n_1 | e^{-\Delta \tau H_b} | n_2 \rangle \langle n_2 | e^{-\Delta \tau H_a} | n_3 \rangle \langle n_3 | e^{-\Delta \tau H_b} | n_4 \rangle \langle n_4 | \ldots \langle n_{2L-2} | e^{-\Delta \tau H_a} | n_{2L-1} \rangle \langle n_{2L-1} | e^{-\Delta \tau H_b} | n_0 \rangle
\]
State of system represented by occupation number paths $n_i(\tau)$
Paths sampled stochastically

Zero Winding
Non-Zero winding
Measurable quantities

\[ \rho_s = \frac{\langle W^2 \rangle}{2dt/\beta} \]

\[ \mu(N) = E(N + 1) - E(N) \]

\[ j(\tau) = \sum_{i=1}^{N_b} [x(i, \tau + 1) - x(i, \tau)] \]

\[ \mathcal{J}(\tau) = \langle j(\tau)j(0) \rangle \]

\[ \mathcal{J}(\omega) = \sum_{\tau} e^{i\omega \tau} \mathcal{J}(\tau) \]

\[ \mathcal{J}(\omega \rightarrow 0) = \frac{1}{\beta} \langle W^2 \rangle \]

\[ S(k) = \sum_r e^{ikr} \langle n(r_0)n(r_0 + r) \rangle \]
Stochastic Series Expansion\(^3\)

Express Hamiltonian as sum of diagonal and non-diagonal operators on bonds of lattice

\[
H = \sum_i (H_{Ui} + H_{Ji})
\]

\[
H_{Ui} = Un_i(n_i - 1) - \mu n_i
\]

\[
H_{Ji} = -J(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i)
\]

Expand partition function in powers of \( H \)

\[
Z = \text{Tr} \ e^{-\beta H} = \sum_\alpha \sum_n \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle.
\]

Insert/remove operators stochastically, satisfying detailed balance.

Considerable similarities with (advanced) world-line algorithms.

Advantages over our (older) world-line implementation:

- Loop updates (reduce autocorrelation times).
- Greens function measurements possible.

Phase diagram

- For $L=64, U=4J$
  - $\rho = N_b / L$
  - $\mu$

- For $\beta=2, U=20t$
  - $L=16, N_b=15$
  - $\Im(\omega)$

- For $\beta=2, U=20t$
  - $L=16, N_b=16$
  - $\Im(\omega)$
Quantum Phase Transition

\[ \kappa = \frac{\partial \rho}{\partial \mu} \rightarrow |\mu - \mu_c|^{-\nu/2} \text{ as } \mu \rightarrow \mu_c \]

\[ \rho_s \sim |\rho - \rho_{Mott}|^{z-d} \]

System sizes ranging from \( L = 16 \) to \( L = 256 \)

Quantum phase transition!

\( z = 2, \quad \nu = 1 \)

\( \beta=2, \ t=1, \ V_0=20 \)

slope = 1.02
One dimensional trapped Boson Hubbard model

No globally incompressible Mott plateau in the trapped system!
As a whole, the system is always compressible.

Local compressibility

Several possible definitions of local compressibility. Simplest:

\[ \kappa_i = \frac{\partial n_i}{\partial \mu_i} \]

No evidence of \( \kappa \) diverging: No quantum phase transition
$\rho$ and $\kappa$ profiles: Fixed $U=4.5$

Local Density $\rho(x)$

Local Compressibility $\kappa(x) = \frac{\partial \rho(x)}{\partial \mu(x)}$

Mott regions always co-exist with SF
$\rho$ and $\kappa$ profiles: Fixed $N_b = 50$

As $U$ is increased, the system **gradually** crosses over to Mott:

No quantum phase transition.
A: $\rho = 1$ Mott
B: SF in center + $\rho = 1$ Mott
C: $\rho = 2$ Mott + SF + $\rho = 1$ Mott
D: SF in center + $\rho = 2$ Mott + SF + $\rho = 1$ Mott
E: SF

The trapped one dimensional bosonic Hubbard model does not exhibit quantum critical behavior like the uniform system.
Visibility Experiments

\[ \mathcal{V} = \frac{S_{\text{max}} - S_{\text{min}}}{S_{\text{max}} + S_{\text{min}}}. \]

\( S_{\text{max}} (S_{\text{min}}) \) are \( \max(\min) \) of momentum distribution,

\[ S(k) = \frac{1}{L} \sum_{j,l} e^{i k \cdot (r_j - r_1)} \langle a_j^\dagger a_l \rangle. \]

- Optical lattice depth \( (U) \) increases: visibility decreases.
- Special values of \( U \): \( \mathcal{V} \) displays “kinks” then decreases again.
- Reflects density redistribution: SF shells transform to MI regions.\(^4\)

QMC Simulations in d=1
Density Profiles and Visibility

Simplest case: density \( n < 2 \). Only Mott domains with \( n = 1 \).

First kink: MI plateau emerge at sides of central SF, \( U = 6.3t \).
Second kink: full MI domain in middle of trap, \( U = 7.1t \).

Experimental control parameter: \((\text{lattice depth})/(\text{recoil energy})\).
\( U/t \) depends exponentially on this quantity.

Unexpected feature: freezing of the density profiles.
Comparedly Featureless.

Does Exhibit signature of Mott Transition at $U \approx 4.5t$.

Visibility begins to decrease from $\nu = 1$. 
Further Signatures of Pause in Density

Difference in densities between $U$ and $U + \delta U$

$6.40 \gtrsim U$: $d\rho(x)/dx < 0$ center; $d\rho(x)/dx > 0$ shoulders.

$6.80 \gtrsim U \gtrsim 6.40$: $d\rho(x)/dx \sim 0$ everywhere.

$U \gtrsim 6.80$: $d\rho(x)/dx < 0$ center; $d\rho(x)/dx > 0$ shoulders.
Pause in the "central density" $\sum_{i=28}^{52} \rho(i)$. Coincides with the plateau-like behavior of $\mathcal{V}$.

6.3 < $U$ < 6.8: bosons no longer pushed out of central regions even though center is compressible SF!

Explanation: Emerging MI domains at the sides trap SF. $U/t$ must increase finite amount before particle transfer.
In interval $U/t = 6.3–6.8$ different pieces of energy pause:

- **Total trapping energy** $E_T$.
- **Interaction energy** $E_P$.
- **Chemical potential** $\mu$.
- **Ratio of potential to kinetic energy**, $\gamma = |E_P/E_K|$.

Total energy (not shown) increases continuously. Decrease in magnitude of the (negative) kinetic energy.
Visibility for System with $\rho = 2$ Mott Lobe

Up to $U/t \sim 13$, $\nu$ is similar to lower density.

Above $U/t = 13$, additional structure.

Visibility kinks from redistribution between $n = 2$ and $n = 1$ MI
(Not from the formation of new SF or MI regions.)
Redistribution occurs discontinuously in $U$. 
Density Profiles for System with $\rho = 2$ Mott Lobe

Visibility structures at $U = (11 - 12)t$ associated with $\rho = 1$ MI shoulder development, and appearance of $\rho = 2$ MI at trap center. Further features in $\nu$ for $U \gtrsim 20$ upon breakup of $\rho = 2$ MI.
Energetics for System with $\rho = 2$ Mott Lobe

Trap center density larger than one (large double occupancy):

- $\gamma$ and $E_P$ increase with $U/t$.
- $\gamma$ reflects the jumps produced by particle redistribution.
- Total energy of the system ($E_S$) increases continuously.
CONCLUSIONS

Equilibrium Phase Diagram of Confined Bosons
- Mott regions always coexist with SF.
- No quantum phase transition, in contrast to uniform case.

“Pause” in Evolution with On-Site Repulsion $U$
- Density distribution constant even when $U$ increases by $t/2$.
- Emergence of static behavior caused by formation of MI “shoulders”
  Transfer of bosons to outer parts of system blocked.

Visibility
- Visibility behaves similar to experiment.
- Kinks: Redistribution of density between MI and SF regions.